

11/365,008

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enhanced
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Applications
NEWS 7 OCT 24 CHEMLIST enhanced with intermediate list of
pre-registered REACH substances
NEWS 8 NOV 21 CAS patent coverage to include exemplified prophetic
substances identified in English-, French-, German-,
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NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
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FILE 'HOME' ENTERED AT 19:20:55 ON 08 DEC 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:21:39 ON 08 DEC 2008
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STRUCTURE FILE UPDATES: 7 DEC 2008 HIGHEST RN 1081539-86-7
DICTIONARY FILE UPDATES: 7 DEC 2008 HIGHEST RN 1081539-86-7

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=>

Uploading C:\Program Files\Stnexp\Queries\10540993e.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 19:22:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 471 TO ITERATE

100.0% PROCESSED 471 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8118 TO 10722

PROJECTED ANSWERS: 1709 TO 3011

L2 50 SEA SSS SAM L1

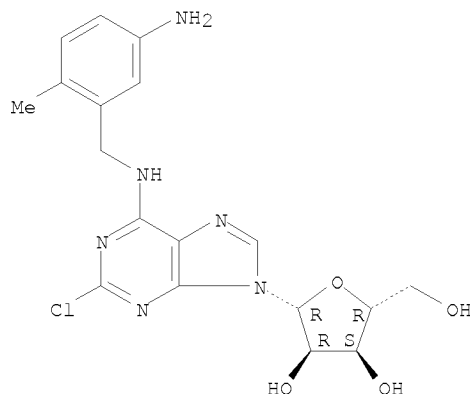
=> d scan

L2 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Adenosine, N-[(5-amino-2-methylphenyl)methyl]-2-chloro- (9CI)

MF C18 H21 Cl N6 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Program Files\Stnexp\Queries\10540993f.str

L3 STRUCTURE UPLOADED

=> s l3

SAMPLE SEARCH INITIATED 19:31:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 397 TO ITERATE

100.0% PROCESSED 397 ITERATIONS

39 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 6745 TO 9135

PROJECTED ANSWERS: 406 TO 1154

L4 39 SEA SSS SAM L3

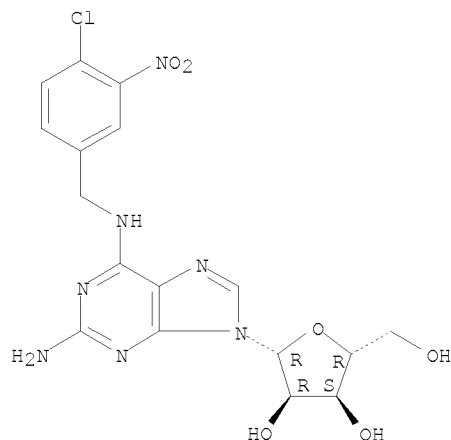
=> d scan

L4 39 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Adenosine, 2-amino-N-[(4-chloro-3-nitrophenyl)methyl]- (9CI)

MF C17 H18 Cl N7 O6

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l4 full

FULL SEARCH INITIATED 19:32:27 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 7566 TO ITERATE

100.0% PROCESSED 7566 ITERATIONS

862 ANSWERS

SEARCH TIME: 00.00.01

L5 862 SEA SSS FUL L3

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.18

186.39

FILE 'CAPLUS' ENTERED AT 19:32:31 ON 08 DEC 2008

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FILE COVERS 1907 - 8 Dec 2008 VOL 149 ISS 24
FILE LAST UPDATED: 7 Dec 2008 (20081207/ED)

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=> s 15

L6 86 L5

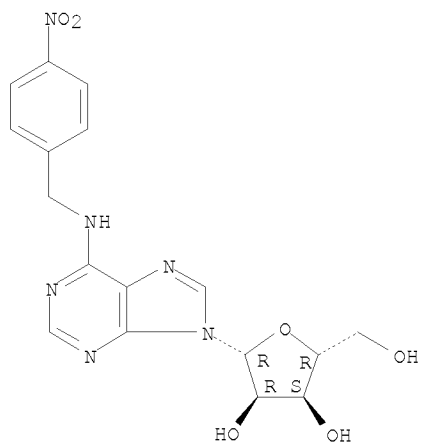
=> d bib abs hitstr 80-86 l6

L6 ANSWER 80 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:557754 CAPLUS
DN 83:157754
OREF 83:24691a,24694a
TI Synthesis and biological activities of some N6-(nitro- and -aminobenzyl)adenosines
AU Dutta, Shib P.; Tritsch, George L.; Cox, Clifford; Chheda, Girish B.
CS Gen. Clin. Res. Cent., Roswell Park Mem. Inst., Buffalo, NY, USA
SO Journal of Medicinal Chemistry (1975), 18(8), 780-3
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB Of 12 title compds., prepared by direct alkylation of adenosine [58-61-7] by a benzyl bromide derivative to give the N1-derivative followed by rearrangement in base, or nucleophilic displacement of Cl in 6-chloropurine nucleosides with an amine, several were inhibitors of adenosine aminohydrolase [9026-93-1] and equal to or more active than N6-benzyladenosine [4294-16-0] as growth inhibitors of leukemia L1210 cells. The highest affinity for the substrate binding site of the enzyme was shown by N6-p-nitrobenzyladenosine (I) [40297-54-9] and N6-p-nitrobenzyl-2'-deoxyadenosine (II) [56527-33-4], which were also relatively nontoxic. 2-Amino-6-p-nitrobenzylamino-9-(β -D-ribofuranosyl)purine (III) [56527-38-9] and 2-amino-6-p-nitrobenzylaminopurine (IV) [56527-39-0] were better inhibitors of L1210 cells than N6-benzyladenosine.
IT 40297-54-9P 40896-40-0P 40896-43-3P
40958-96-1P 56527-36-7P 56527-38-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. activity of)
RN 40297-54-9 CAPLUS
CN Adenosine, N-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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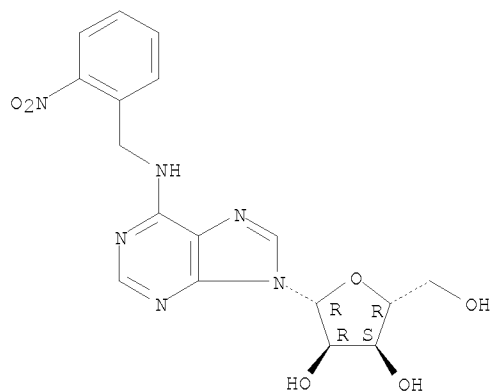
11/365,008



RN 40896-40-0 CAPLUS

CN Adenosine, N-[(2-nitrophenyl)methyl]- (CA INDEX NAME)

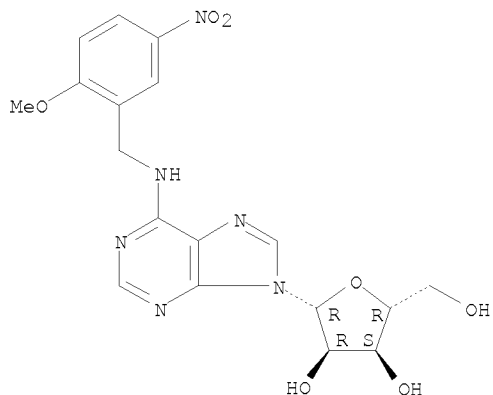
Absolute stereochemistry.



RN 40896-43-3 CAPLUS

CN Adenosine, N-[(2-methoxy-5-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



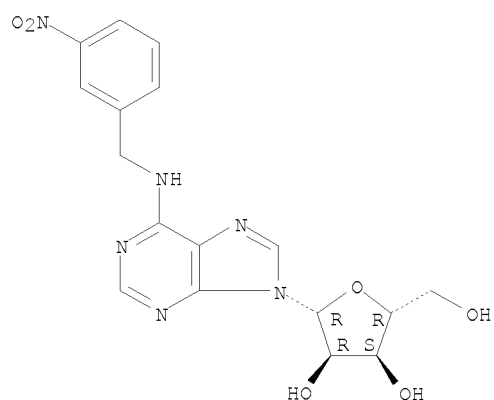
RN 40958-96-1 CAPLUS

CN Adenosine, N-[(3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

McIntosh

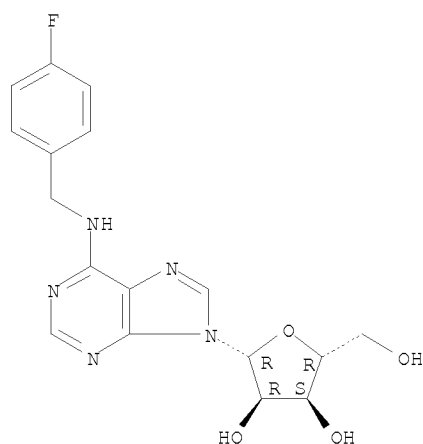
11/365,008



RN 56527-36-7 CAPLUS

CN Adenosine, N-[(4-fluorophenyl)methyl]- (CA INDEX NAME)

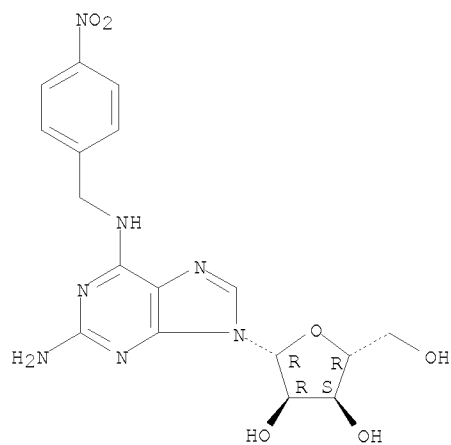
Absolute stereochemistry.



RN 56527-38-9 CAPLUS

CN Adenosine, 2-amino-N-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

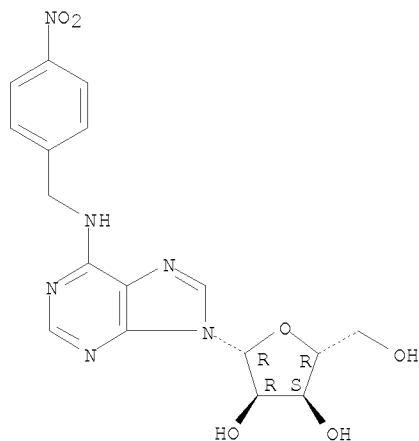


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L6 ANSWER 81 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1973:413413 CAPLUS
DN 79:13413
OREF 79:2119a,2122a
TI Inhibitors of nucleoside and nucleotide metabolism
AU Henderson, J. F.; Paterson, A. R. P.; Caldwell, I. C.; Paul, B.; Chan, M. C.; Lau, K. F.
CS Cancer Res. Unit, Univ. Alberta, Edmonton, AB, Can.
SO Cancer Chemotherapy Reports, Part 2 (1973), 3(1), 71-85
CODEN: CCSUBJ; ISSN: 0069-0120
DT Journal
LA English
AB A total of 164 purine and pyrimidine derivs. and analogs were screened for inhibition of nucleoside and nucleotide metab in 4 test systems. Among a number of potent inhibitors identified, N6-(3-methyl-2-butenyl)-adenosine [7724-76-7] and 4-(dimethylamino)-7- β -D-ribofuranosyl-7H-pyrrolo[2,3-d]pyrimidine (I) [20371-00-0] inhibited de novo purine biosynthesis in incubated Ehrlich ascites tumor cells, α -(9-amino-9H-purin-9-yl)- α' -(hydroxymethyl)diglycolaldehyde-bis(phenylhydrazine) (II) [40297-52-7] inhibited adenine phosphoribosyltransferase [9027-80-9] from Ehrlich ascites tumor cells, 4-amino-5-iodo-7- β -D-ribofuranosyl-7H-pyrrolo[2,3-d]pyrimidine [24386-93-4] inhibited adenine kinase [9027-72-9] activity in tumor cell exts., and 2-amino-6-[(p-fluorobenzyl)thio]-9- β -D-ribofuranosyl-9H-purine (III) [40297-53-8] and N6-(p-nitrobenzyl)-adenosine [40297-54-9] inhibited nucleoside transport (inosine synthesis) in incubated human erythrocytes.
IT 40297-54-9
RL: BIOL (Biological study)
(inosine formation by erythrocytes in response to)
RN 40297-54-9 CAPLUS
CN Adenosine, N-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



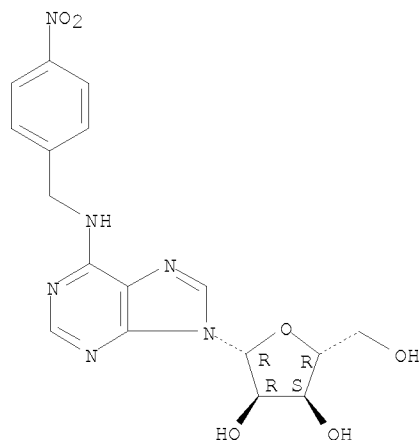
L6 ANSWER 82 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1973:124846 CAPLUS
DN 78:124846
OREF 78:20071a,20074a
TI N-Benzyladenosine derivatives
IN Kampe, Wolfgang; Fauland, Erich; Thiel, Max; Juhran, Wolfgang; Stork, Harald
PA Boehringer Mannheim G.m.b.H.
SO Ger. Offen., 20 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2136624	A	19730208	DE 1971-2136624	19710722

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GB 1340643	A	19731212	GB 1972-33537	19720618
US 3845035	A	19741029	US 1972-271098	19720712
ZA 7204891	A	19730530	ZA 1972-4891	19720717
CH 569035	A5	19751114	CH 1975-10617	19720719
CH 570420	A5	19751215	CH 1972-10795	19720719
NL 7210023	A	19730124	NL 1972-10023	19720720
CA 979891	A1	19751216	CA 1972-147625	19720720
SU 539532	A3	19761215	SU 1972-1812966	19720720
FR 2146493	A1	19730302	FR 1972-26450	19720721
AT 317446	B	19740826	AT 1972-6288	19720721
AT 790673	A	19750415	AT 1973-7906	19720721
PRAI DE 1971-2136624	A	19710722		
GI	For diagram(s), see printed CA Issue.			
AB	Thirty-three title compds. (I; X = NHCH ₂ C ₆ H ₅ -nRn; R: = Cl, OH NH ₂ or Br; Rn = e.g. 2-OH, 3,2-HOMe, 2,5 HOCl, 2,4- HOCl) were prepared by reaction of I (X = Cl) containing free or acetyl group-protected OH-groups with H ₂ NCH ₂ C ₆ H ₅ -nRn or from the adenosine derivative and ClCH ₂ C ₆ H ₅ nRn. I had circulatory and antilipemic effects.			
IT	40297-54-9P 40896-40-0P 40896-41-1P 40896-42-2P 40896-43-3P 40896-45-5P 40896-46-6P 40896-47-7P 40896-48-8P 40896-49-9P 40896-50-2P 40896-51-3P 40896-52-4P 40896-53-5P 40958-96-1P 40958-97-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	40297-54-9 CAPLUS			
CN	Adenosine, N-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)			

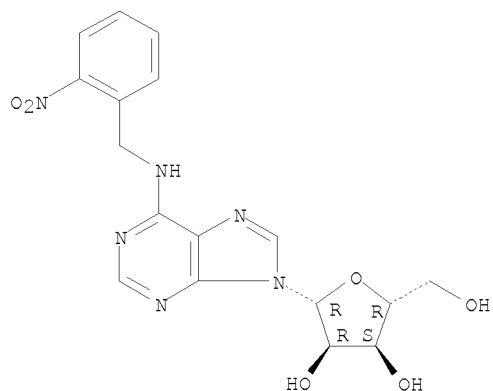
Absolute stereochemistry.



RN 40896-40-0 CAPLUS
CN Adenosine, N-[(2-nitrophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

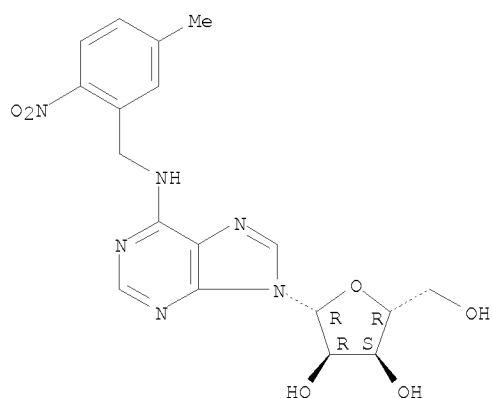
11/365,008



RN 40896-41-1 CAPLUS

CN Adenosine, N-[(5-methyl-2-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

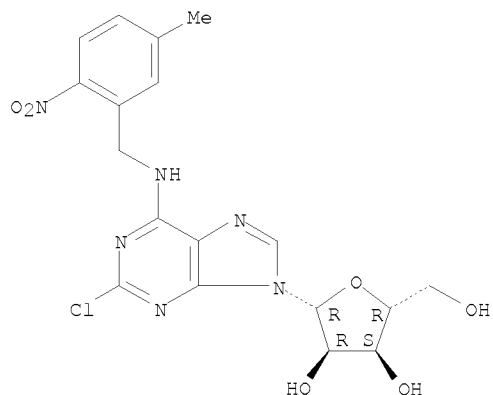
Absolute stereochemistry.



RN 40896-42-2 CAPLUS

CN Adenosine, 2-chloro-N-[(5-methyl-2-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



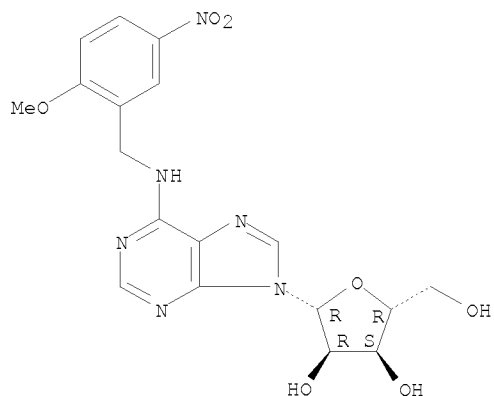
RN 40896-43-3 CAPLUS

CN Adenosine, N-[(2-methoxy-5-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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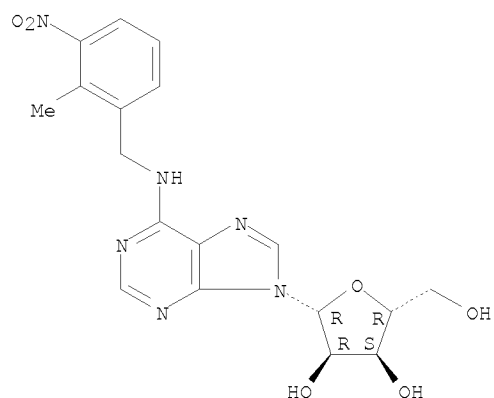
11/365,008



RN 40896-45-5 CAPLUS

CN Adenosine, N-[(2-methyl-3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

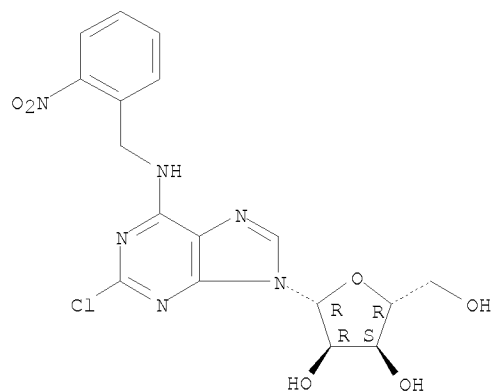
Absolute stereochemistry.



RN 40896-46-6 CAPLUS

CN Adenosine, 2-chloro-N-[(2-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



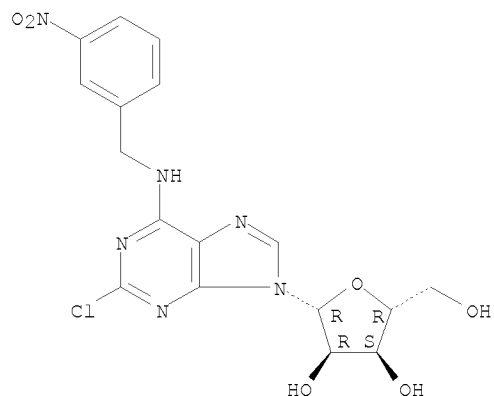
RN 40896-47-7 CAPLUS

CN Adenosine, 2-chloro-N-[(3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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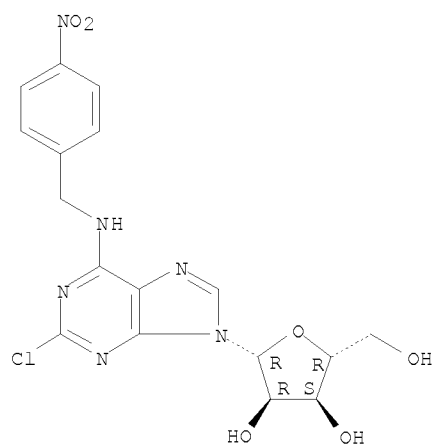
11/365,008



RN 40896-48-8 CAPLUS

CN Adenosine, 2-chloro-N-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

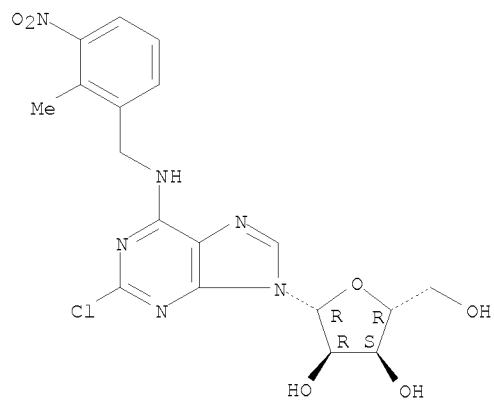
Absolute stereochemistry.



RN 40896-49-9 CAPLUS

CN Adenosine, 2-chloro-N-[(2-methyl-3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



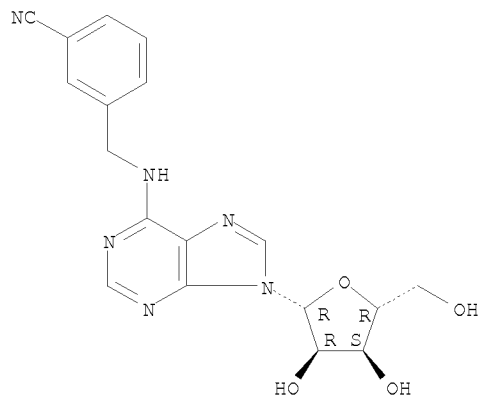
RN 40896-50-2 CAPLUS

CN Benzonitrile, 3-[[[9-beta-D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

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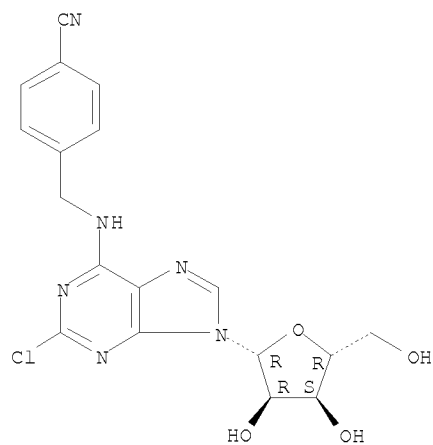
11/365,008

Absolute stereochemistry.



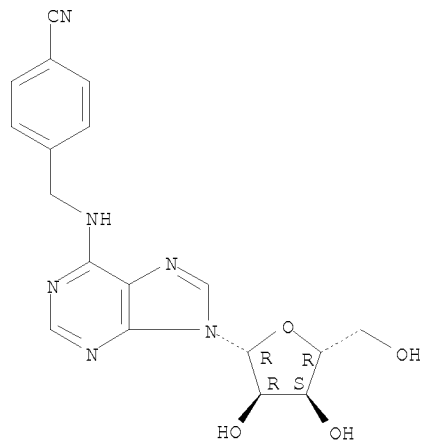
RN 40896-51-3 CAPLUS
CN Benzonitrile, 4-[[(2-chloro-9-beta-D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 40896-52-4 CAPLUS
CN Adenosine, N-[(4-cyanophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

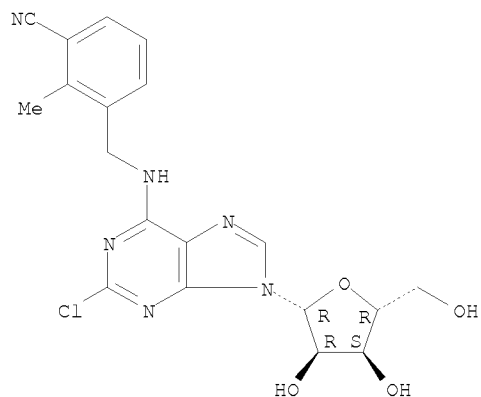


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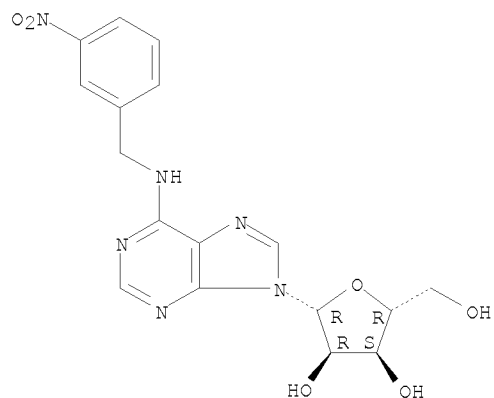
RN 40896-53-5 CAPLUS
CN Benzonitrile, 3-[[[2-chloro-9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



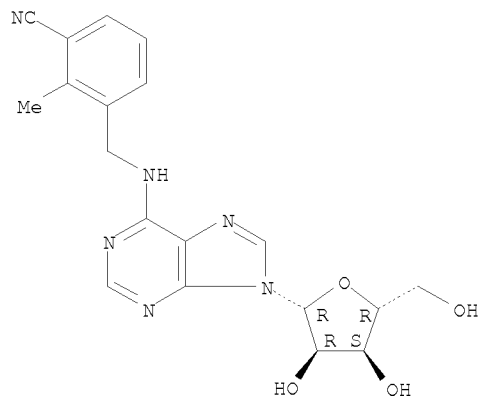
RN 40958-96-1 CAPLUS
CN Adenosine, N-[(3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 40958-97-2 CAPLUS
CN Adenosine, N-[(3-cyano-2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

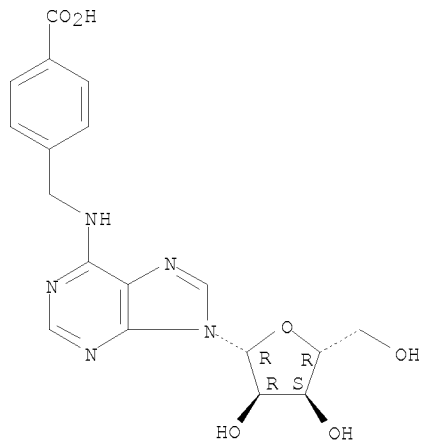


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L6 ANSWER 83 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1972:502139 CAPLUS
 DN 77:102139
 OREF 77:16847a,16850a
 TI N-(Acylbenzyl- and -phenethyl)adenosines
 IN Kampe, Wolfgang; Fauland, Erich; Stork, Harald; Juhran, Wolfgang;
 Dietmann, Karl
 PA Boehringer Mannheim G.m.b.H.
 SO Ger. Offen., 20 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2059922	A	19720615	DE 1970-2059922	19701205
	US 3817981	A	19740618	US 1971-199727	19711117
	SU 469253	A3	19750430	SU 1971-1723201	19711130
	SU 506294	A3	19760305	SU 1971-1913745	19711130
	NL 7116563	A	19720607	NL 1971-16563	19711202
	GB 1313290	A	19730411	GB 1971-56024	19711202
	CH 567044	A5	19750930	CH 1971-17633	19711202
	CH 573445	A5	19760315	CH 1975-8318	19711202
	FR 2116517	A5	19720713	FR 1971-43419	19711203
	FR 2116517	B1	19750801		
	ZA 7108104	A	19720927	ZA 1971-8104	19711203
	AU 7136493	A	19730607	AU 1971-36493	19711203
	HU 163670	B	19731027	HU 1971-B01334	19711203
	AT 314094	B	19740325	AT 1971-10436	19711203
	CA 960655	A1	19750107	CA 1971-129319	19711203
	AT 323335	B	19750710	AT 1971-323335	19711203
PRAI	DE 1970-2059922	A	19701205		
GI	For diagram(s), see printed CA Issue.				
AB	Forty-five title compds. (I, Y = X, 2-R(R1)C6H39CH2)nNH; n = 1,2; R = 3- or 4-carboxy, -alkoxycarbonyl, -carbamoyl, -allylcarbamoyl; R1 = H, Me; R2 = H, Cl, OH) (II), useful as hypolipemic agents with effects on circulation, were prepared by reaction of the corresponding I (Y = Cl) (III) with X, 2-R(R1)C6H3(CH2)nNH2 and subsequent saponification or amidation. Thus, refluxing III (R2 = H) and 3-EtO2C-C6H4CH2CH2NH2.HCl in EtOH in the presence of Et3N for 3 hr gave 65% II (n = 2, R = 3-EtO2C, R1 = R2 = H), which was heated in EtOH at 120° for 15 hr with NH3 to give 64% II (n = 2, R = 3-H2NCO, R1 = R2 = 5h).				
IT	38823-65-3P 38823-66-4P 38823-67-5P 38823-68-6P 38823-69-7P 38823-72-2P 38823-73-3P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	38823-65-3	CAPLUS			
CN	Benzoic acid, 4-[[[9-β-D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)				

Absolute stereochemistry.

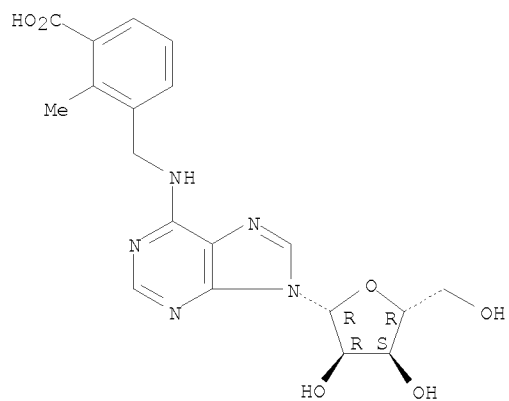


11/365,008

RN 38823-66-4 CAPLUS

CN Benzoic acid, 2-methyl-3-[[[(9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

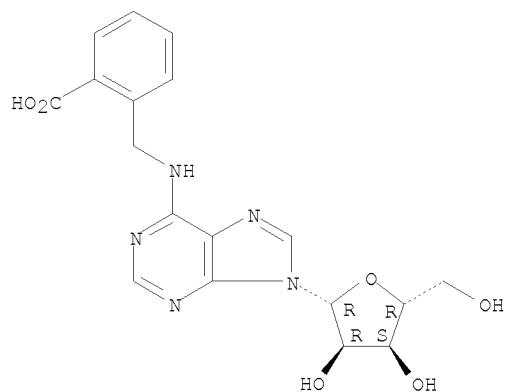
Absolute stereochemistry.



RN 38823-67-5 CAPLUS

CN Benzoic acid, 2-[[[(9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

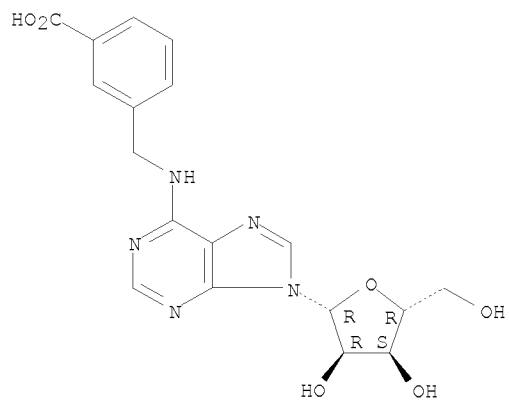
Absolute stereochemistry.



RN 38823-68-6 CAPLUS

CN Benzoic acid, 3-[[[(9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



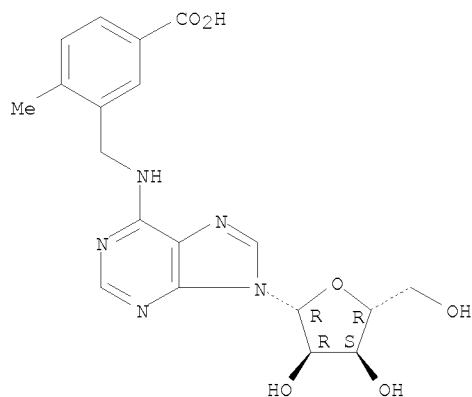
McIntosh

11/365,008

RN 38823-69-7 CAPLUS

CN Benzoic acid, 4-methyl-3-[[[(9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

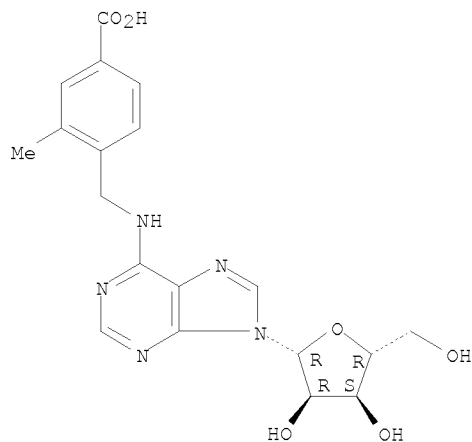
Absolute stereochemistry.



RN 38823-72-2 CAPLUS

CN Benzoic acid, 3-methyl-4-[[[(9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

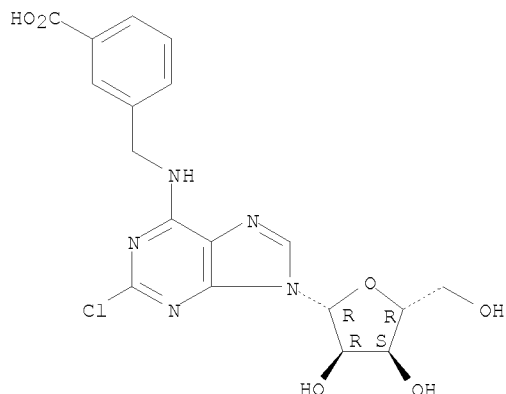


RN 38823-73-3 CAPLUS

CN Benzoic acid, 3-[[[(2-chloro-9- β -D-ribofuranosyl-9H-purin-6-yl)amino]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

McIntosh



L6 ANSWER 84 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1971:541121 CAPLUS

DN 75:141121

OREF 75:22273a,22276a

TI Coronary dilating N6-benzyladenosines

IN Kampe, Wolfgang; Fauland, Erich; Thiel, Max; Dietmann, Karl; Juhran, Wolfgang

PA Boehringer Mannheim G.m.b.H.

SO Ger. Offen., 10 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2007273	A	19710826	DE 1970-2007273	19700218
	SU 399134	A3	19730927	SU 1971-1616102	19710129
	US 3781273	A	19731225	US 1971-112424	19710203
	ES 388194	A1	19730501	ES 1971-388194	19710212
	NL 7102026	A	19710820	NL 1971-2026	19710216
	DK 123357	B	19720612	DK 1971-694	19710216
	HU 162739	B	19730428	HU 1971-B01274	19710216
	CH 549596	A	19740531	CH 1971-2208	19710216
	CH 549600	A	19740531	CH 1974-2849	19710216
	CA 953714	A1	19740827	CA 1971-105563	19710216
	ZA 7101030	A	19711124	ZA 1971-1030	19710217
	FR 2081524	A5	19711203	FR 1971-5318	19710217
	FR 2081524	B1	19740927		
	AT 306251	B	19730410	AT 1971-1378	19710217
	AT 313483	B	19740225	AT 1972-1233	19710217
	JP 51016440	B	19760524	JP 1971-7691	19710218
	GB 1279946	A	19720628	GB 1971-1279946	19710419
PRAI	DE 1970-2007273	A	19700218		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I, where R = Me, MeS, or MeO, R1 = 5-Me, 5-Cl, 5-MeO, 5-iso-Pr, 5-F, 5-tert-Bu, 3-Me, or 3-Cl) were prepared wither by amination of the 6-chloro derivative or by N1-substitution of adenosine followed by alkaline rearrangement. Thus, 9-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-6-chloropurine, 2,5-Me2C6H3CH2NH2, and Et3N in iso-PrOH was refluxed 3 hr and the protective Ac groups cleaved by NaOMe to give 61% I (R = Me, R1 = 5-Me). Similarly prepared were 11 other I.

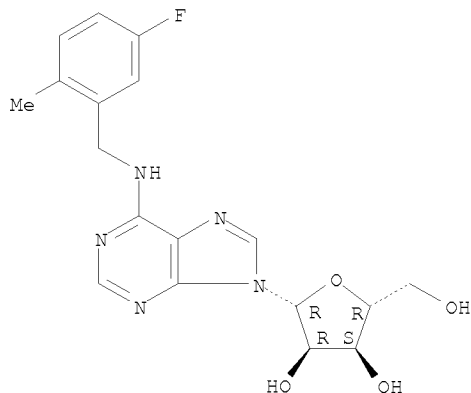
IT 34349-37-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34349-37-6 CAPLUS

CN Adenosine, N-[(5-fluoro-2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 85 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1970:21921 CAPLUS

DN 72:21921

OREF 72:4037a,4040a

TI 2-Aminoadenosine derivatives with cardiac activity

IN Koch, Klaus; Fauland, Erich; Stach, Kurt; Thiel, Max; Schaumann, Wolfgang; Dietmann, Karl

PA Boehringer, C. F., und Soehne G.m.b.H.

SO S. African, 25 pp.

CODEN: SFXAB

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 6805477		19690128		
	DE 1670265			DE	
	FR 1587681			FR	
	GB 1164580			GB	
	US 3590029		19710629	US	19680822
PRAI	DE		19670825		

GI For diagram(s), see printed CA Issue.

AB The title compds. [I, R = NHR1 (II), R1 = PhCH2, (Ph)MeCHCH2, Pr, o-ClC6H4CH2, iso-Bu, o-MeC6H4CH2, o-F3CC6H4, furf uryl, 3,4-(MeO)2C6H3CH2CH2, PhCH(OH)CHMe, PhCH(CO2H), allyl, cyclohexyl, 2-hydroxy-3-(m-cresoxy)propyl, 2-phenylcyclopropyl, 1-adamantyl, 2-(β-indolyl)ethyl, 2-indanyl, Bu, benzhydryl, 2,4-Cl2C6H3CH2, p-HOC6H4CH2CH2, o-PhOC6H4CH2, o-MeOC6H4CH2, PhCH2CH2, 3,5-(MeO)2C6H3CH2, p-ClC6H4CH2, 2-ethylhexyl, m-FC6H4CH2, HOCH2CH2, PhCHMe, 2-phenylcyclohexyl, PhOCH2CHMe, 2-hydroxy-3-(α-naphthoxy)propyl, Me2C:CHCH2, p-O2NC6H4-CHOHCH2, p-MeSO2NHC6H4CH2 or EtCHCH2OH] are prepared from I (R = Br) (III) and appropriate amines. II has cardiac and circulatory activities. For example, a mixture of 5 g III, 1.71 g PhCH2NH2 and 2.92 g Et3N in 50 ml Me2CHOH was refluxed 3 hr to give 29% II (R1 = PhCH2), m. 92° (decomposition).

2',3',5'-Tri-O-acetyl-2-amino-6-chloronebularin was also used in place of III, and the resulting substitution product was hydrolyzed to give II.

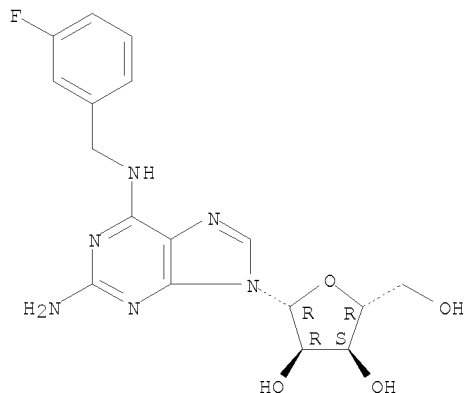
IT 26775-38-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 26775-38-2 CAPLUS

CN Adenosine, 2-amino-N-[(3-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 86 OF 86 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1969:115505 CAPLUS

DN 70:115505

OREF 70:21591a,21594a

TI N6-Aralkyl adenosine derivatives

IN Thiel, Max; Stach, Kurt; Jahn, Werner; Schaumann, Wolfgang; Dietmann, Karl

PA Boehringer, C. F., und Soehne G.m.b.H.

SO S. African, 15 pp.

CODEN: SFXXAB

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 6707414		19680502		
	DE 1670171			DE	
	FR 1550512			FR	
	GB 1145789			GB	
	US 3506643		19700414	US	19671018
PRAI	DE		19661209		
	DE		19670711		

OS MARPAT 70:115505

GI For diagram(s), see printed CA Issue.

AB The title compds. (1), where halogen, alkyl, alkoxy, F3C or alkylthio, or two substituents may be H or a methylenedioxy, are prepared from the corresponding D-ribosides and benzylamines, or from the corresponding N'-substituted adenosine derivs. Thus, 8.2 g. tri-O-acetyl-6-chloro-9-β-D-ribose-9-H-purine and 7.2 g. 2-ClC6H4CH2NH2 in 120 cc. iso-PrOH were refluxed 2 hrs., worked up and the residue dissolved in 100 cc. MeOH, 10 cc. N NaOH solution added and the mixture refluxed 1 hr. to yield 4 g. I (R = 2-Cl), m. 182-3°. The following I were similarly prepared (R and m.p. given): 3,4-Cl2, 182-3°; 4-MeO, 146-7°; 3,4(MeO)2, 135-6°; 3,4,5-(MeO)3, 118-19°; 2,6-Cl2, 207-9°; 4-Cl, 174-5°; 3-Cl, 168-9°; 2-MeO, 147-8°; 2-Me, 157-8°; 3,5-(MeO)2, 191-2°; 2-MeS, 127-8°; 2-F3C, 160-1°; and 3-F3C, 111-12°. To a suspension of 10 g. 2',3'-O-isopropylideneadenosine in 200 cc. MeCN, 10 g. p-BrC6H4Br was added and the mixture refluxed 24 hrs. with stirring. The precipitate which formed was filtered off, dissolved in 150 cc. MeOH and an equal volume 2N NaOH solution was added. The mixture was heated on a steam bath 20 min., extracted with CHCl3, evaporated, and the residue dissolved in 200 cc. HCO2N. Water was added until the mixture became cloudy. The mixture was left standing 1 day at ambient temperature, after which it was evaporated in vacuo, and the residue made weakly alkaline with an aqueous solution of concentrated NH3 to yield 5.8 g. I (R = 4-Br), m. 168-9°. I exhibit an effect on blood vessels and circulation.

IT 23666-27-5P

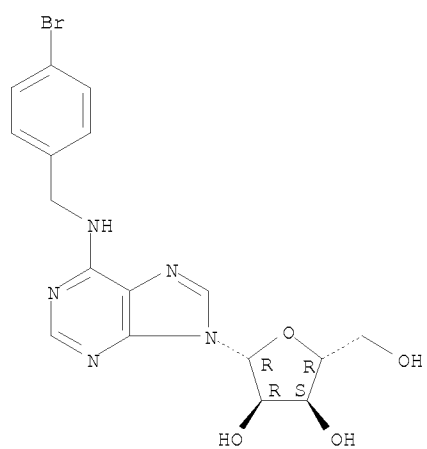
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23666-27-5 CAPLUS

CN Adenosine, N-[(4-bromophenyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

11/365,008



McIntosh